AEOSR-TR- 94 0390

Approved for public release; distribution unlimited.

# AD-A281 369

Report: Grant No. AFOSR-91-0137

RESONANT CHARGE TRANSFER IN HYPERTHERMAL ATOMIC AND MOLECULAR ION-SURFACE COLLISIONS

Barbara H. Cooper Laboratory of Atomic and Solid State Physics Clark Hall Cornell University Ithaca, New York 14853-2501

Approved for public releases ,
Distribution Unlimited

April 14, 1994

Interim Report for Period: 1 January 1993 - 1 April 1994



Distribution Statement

Prepared for

CHEMICAL AND ATMOSPHERIC SCIENCES PROGRAM

AFOSR/NC Building 410 Bolling AFB

DC 20332-6448

DITE QUALITY INSPECTED 5

94-20726

947

6

177

# REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burgen for this collection of information is estimated to average 1 nour per response, including the time for reviewing instructions, searching earling data sources.

Jathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden. To Washington readquarters hervices. Directorate for information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204. Arlington, VA. 22202-4307, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC. 20503.

	AGENCY USE ONLY (Leave blank)	2. REPORT DATE 14 April 1994		D DATES COVERED /01/01 - 94/04/01							
4.	TITLE AND SUBTITLE		HAMOOL	5. FUNDING NUMBERS							
	Resonant Charge Transfer and Molecular Ion-Surfac	121102F 2303									
6.	AUTHOR(S)	3305									
ľ	B.H. Cooper			BS							
7.	PERFORMING ORGANIZATION NAME(	S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION							
	LASSP			REPORT NUMBER							
	531 Clark Hall										
	Cornell University Ithaca, NY 14853-2501			160 SR-JR- 94 0390							
	ıtnaca, NI 14033~23U1										
9.	SPONSORING/MONITORING AGENCY	NAME(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER							
	AFOSR/NC			AGENCT REPURT NUMBER							
	Building 410		AFOSR-91-0137								
	Bolling AFB Washington, DC 20332-644	<b>≒ &amp;</b>									
	MAJ Erstiell.	<del></del>									
11	I. SUPPLEMENTARY NOTES										
12	a. DISTRIBUTION / AVAILABILITY STAT	EMENT	**** <del>*</del> * -	12b. DISTRIBUTION CODE							
	Approved for public re	elease; distribution	unlimited.								

13. ABSTRACT (Maximum 200 words)

We are investigating the interactions of hyperthermal energy (few to several hundred eV) atomic ions with metal surfaces, focusing on ion-surface charge exchange processes. For Li<sup>+</sup> scattering from alkali-covered Cu(001), we have measured branching ratios for Li<sup>+</sup>, Li<sup>-</sup> and ground- and excited-state Li<sup>o</sup> in the scattered flux. These results are interpreted using a state-of-the art multi-channel charge transfer code developed by Brad Marston. Using this code, we have gained important insights into the dynamics of multi-channel charge transfer processes. We are extending these studies to higher-lying excited states of Li, excited state formation in Na scattering, and multi-channel charge transfer in O scattering. For Na<sup>+</sup> scattering from clean Cu(001) we have observed trajectory-dependent charge transfer in which the charge transfer probability is dependent on the collisional history of the particle; evidence is found for modification of the neutralisation due to defect formation that can occur in certain types of collisions with the surface. We plan to study trapping behavior for hyperthermal energy alkalis and oxygen incident on metal surfaces.

14. SUBJECT TERMS Charge	15. NUMBER OF PAGES		
<pre>ing; Classical Traje Ions; Hyperthermal O Dynamics: Energy Tra</pre>	16. PRICE CODE		
	18. SECURITY CLASSIFICATION OF THIS PAGE		20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL SAR

#### TABLE OF CONTENTS

I.	Summary					•										1
	Research Objectives															
III.	Status of Research .															3
IV.	References				•											9
V.	Figures															11
VI.	Research Participants		•													17
VII.	Publications, book cha	ap	te	rs,	aı	tic	:le	8,	the	ese	s					17
VIII.	Presentations															20

# I. SUMMARY

The objectives of the research program described in this report are to investigate the interactions of hyperthermal energy (10-100 eV) and low energy (keV) ions with clean and adsorbate-covered metal surfaces. A particular emphasis is placed on the study of ion-surface charge exchange processes. Charge exchange, the transfer of electrons between the scattering ion and surface atoms, is an essential step in many gas-surface dynamical processes, such as dissociation, energy transfer, trapping, and adsorption. For understanding surface reactions in the space environment (e.g., surface reactions in low earth orbit) it is of particular interest to understand charge transfer and collision dynamics at 10 eV and lower. The hyperthermal energy range is also widely used in surface processing techniques such as reactive ion etching, ion beam-assisted thin film deposition, and surface modifications by plasma processing and deposition.

Our goal is to obtain experimental information about the basic mechanisms of the charge transfer process. The experiments are accompanied by theoretical calculations to identify the physical properties of the system that influence charge transfer probabilities. Ultimately this knowledge will be integrated with a more complete description of scattering at hyperthermal energies in order to understand the role that charge transfer plays in determining the collision dynamics.

We have obtained results in the following areas, some of which were covered in our progress report submitted in March 1993, and others that will be covered in detail below:

- The development and testing of a time-of-flight spectrometer for energy- and angleresolved detection of neutral and charged low and hyperthermal energy alkalis.<sup>1,2</sup> (Covered in 1993 report.)
- 2. Measured velocity-dependent neutralization probabilities for Li, Na, and K scattering from clean Cu(001). These data were compared to calculated neutralization probabilities derived from a "one-electron" model of the resonant charge transfer process.

  This model, developed by Brako and Newns, describes the relatively simple case where transfer occurs primarily to one electronic level in the scattered particle. This work demonstrates that the neutralization probabilities are very sensitive to the energies and lifetimes of atomic resonances near the surface. The experiments provide im-



Special

- portant experimental tests of charge transfer models, and theoretical calculations of atomic state lifetimes and energies.<sup>3-5</sup> We have also demonstrated that the neutralization probability for 5-1200 eV Na scattering from Cu(001) is sensitive to the component of the scattered particle's velocity that is parallel to the surface. This behavior was initially unexpected and can be understood using a modified version of the one-electron model discussed above. (Covered in 1993 report.)
- 3. In general, charge transfer involves the simultaneous interaction of several atomic states with the surface electronic states. To understand these processes in detail, we have made measurements of branching ratios to different final electronic states for Li<sup>+</sup> scattering from alkali-covered Cu(001) surfaces. In the final state we observed Li<sup>+</sup>, Li<sup>-</sup>, Li(2s) (ground state neutrals), and Li(2p) (excited state neutrals). With theorist Brad Marston from Brown University, we are analyzing these data using a multi-state charge transfer model. Unlike the one-electron model discussed above, this model can treat the case where multiple final states are formed via charge transfer processes. This work provides insights into the dynamics of the multi-channel charge transfer processes. We are developing a monochromator system that will enable us to look for additional excited states in the scattered flux. (Recent progress from this work will be reported below.)
- 4. Results have been obtained for scattering O<sub>2</sub><sup>+</sup> from clean and adsorbate-covered Cu(001), and for scattering of O<sup>+</sup> from clean Cu(001). We have observed the formation of O<sup>-</sup> and O<sub>2</sub><sup>-</sup> resulting from O<sub>2</sub><sup>+</sup> collisions with clean and adsorbate-covered surfaces. Following calibration of our ion detector, we have made quantitative measurements of the O<sup>-</sup>/O<sup>+</sup> yields for O<sup>+</sup> scattering from clean Cu(001). (These results were covered in the 1993 report.) We are analyzing these yields using models developed by Peter Nordlander and Brad Marston. Planned modifications to the alkali neutral detector will enable us to directly detect scattered neutral oxygen, which becomes the dominant channel for the scattered particles at low energies.
- 5. We have observed trajectory-dependent neutralization for Na<sup>+</sup> scattering from clean Cu(001). For 50eV and 7.5eV incident Na energies, we have observed neutralization probabilities that vary from 0.07 to 0.5 for particles that have the same outgoing velocity and angle, but different collisional histories. These results represent the first report of trajectory-dependent neutralization from a clean surface. Modeling indicates that the different surface atomic displacements produced in the different types of collisions can explain the dramatic variation in neutralization with collision type. (Recent progress from this work will be reported below.)
- 6. Ultimately our goal is to incorporate our understanding of charge transfer into a more complete description of the dynamics of scattering at hyperthermal energies, i.e., to determine the role that charge transfer plays in energy transfer to the surface and particle trapping. Below we discuss planned experiments (initially with Na<sup>+</sup>, O<sup>+</sup>, and O<sub>2</sub><sup>+</sup> ions), using the apparatus developed with this grant, that will address these issues.

#### II. RESEARCH OBJECTIVES

Our research objectives under grant number AFOSR-91-0137 are as follows:

- 1. To develop instrumentation for quantitative measurements of branching ratios to different final electronic states of hyperthermal energy atoms and molecules scattered from clean and adsorbate-covered surfaces.
- 2. To use these measured branching ratios to probe basic mechanisms of charge transfer for alkalis scattered from clean copper surfaces. Charge transfer calculations are used to extract information about the energies and lifetimes of atomic electronic resonances near surfaces, and to probe the dynamics of multi-channel charge transfer processes.
- 3. To extend the knowledge we have gained about nonadiabatic charge transfer processes for the relatively simple alkali-Cu systems to more complex systems, such as oxygen scattering from metal surfaces. These latter cases require more sophisticated experimental and theoretical treatments.
- 4. To explore the role that charge transfer plays in influencing the dynamics of hyperthermal scattering from surfaces, in particular particle trapping.

#### III. STATUS OF RESEARCH

Recent results from this research are outlined briefly below and can be found described in more detail elsewhere (relevant references are given).

# Charge Transfer Dynamics in Ion-Surface Collisions - Motivation:

Electron transfer between the particle and surface by one of a number of processes (e.g., resonant electron tunneling, Auger, direct radiative transfer) can result in a change in the particle's charge state.<sup>6</sup> Charge transfer processes are a fundamental step in a number of surface processes, including dissociative chemisorption, trapping, and laser-induced desorption.

Charge transfer processes are also important in understanding the dynamics of ionsurface collisions at hyperthermal energies (i.e., few eV to several hundred eV). A change in charge state, say from positive ion to neutral atom, alters the particle-surface potential and changes the energy transferred to the surface, the energy and angular distributions of the scattered particles, and trapping thresholds and mechanisms. This is particularly true at energies below approximately 50 eV, where the ion-surface image attraction represents a significant fraction of the total scattering potential. In the case of molecular scattering, the same issues apply, with the additional factor that charge transfer can promote dissociation, leading to the production and scattering of molecular fragments.

Charge transfer events are very sensitive to the details of the electronic structure of the specific particle and surface in question. As an atom or molecule approaches a surface, its electronic levels, which are narrow in energy far from the surface, become broadened, shifted, and hybridized resonances near the surface. The lifetimes and energies of these resonances are rapidly varying functions of particle-surface separation z. Thus, at different z, a given resonance is degenerate with different states in the substrate. For example, in the

case of a metal substrate, the energy shift may mean that the resonance lies predominantly above the Fermi level on some parts of the trajectory, and below it on others. The lifetimes and energies of different resonances, and whether they are degenerate with filled or empty states in the substrate, are factors which lie at the root of many particle-surface dynamical interactions, whether they be scattering, adsorption, desorption, etc.<sup>1,6-8</sup> The resonance energies and lifetimes are difficult to calculate<sup>3-5</sup> and difficult to access directly by most experimental techniques. They can, however, be studied by scattering experiments, such as those presented below.

When a particle approaches or leaves the surface at non-zero velocity, at any given instant the system may or may not be in the adiabatic electronic ground state, depending on various time scales in the collisions. In the hyperthermal energy range the time scales of the collisions can be comparable to the time scales of electron transfer (resonance lifetimes) between the particle and surface, making it possible to nonadiabatically populate different final electronic states on the outgoing trajectory. The faster the scattered particle, the closer to the surface (where the lifetimes are shortest) the final electronic state is determined. Thus, the branching ratios to different final electronic states will vary with velocity. In the "standard model" of resonant charge transfer, 9,10 it is assumed that the important velocity component is that which is perpendicular to the surface,  $v_{\perp}$ , since the particle-surface coupling is assumed to be a function of z. For a given incident species, the branching ratios will also be sensitive to changes in the Fermi energy (i.e., changes in the work function  $\Delta\Phi$ ) of the substrate. For example, lowering the work function will change where the Fermi level crossings occur, and may bring higher lying atomic states into resonance with occupied surface states. This latter type of experiment is discussed below.

# Many-body effects in resonant neutralization for Li and Na scattering from alkali-covered Cu(001)

For Li<sup>+</sup> scattering from alkali-covered Cu(001) we have measured branching ratios for scattering into different final electronic states; in particular Li<sup>+</sup>, Li<sup>-</sup>, Li(2s) (neutral ground state), and Li(2p) (neutral excited state).<sup>11-14</sup> In the 1993 interim report, preliminary results were presented. The key results are highlighted here along with recent progress toward modeling these results and extending the measurements.

## Experimental results:

Figure 1 is a plot of the measured probabilities with which an impinging 400eV Li<sup>+</sup> ion scatters from the Cs/Cu(001) surface as a positive ion (P<sup>+</sup>) or a negative ion (P<sup>-</sup>) versus the work function shift induced by the deposition of Cs. <sup>11,12,14</sup> The 400 eV Li<sup>+</sup> ions impinge at an angle of  $\theta_i = 65^{\circ}$ , measured with respect to the surface normal, and along the  $\langle 100 \rangle$  azimuth. The detected particles have been scattered into a final angle of  $\theta_f = 64^{\circ}$ , also measured with respect to the surface normal. For the clean surface, P<sup>+</sup> is 0.67 ( $v_{\perp} = 0.02$  a.u.). As the work function decreases from its clean surface value of  $\Phi$ =4.59 eV ( $\Delta\Phi$  = 0.0 eV) to a value of about 2.6 eV ( $\Delta\Phi$  ≈ -2.0 eV), P<sup>+</sup> decreases, with a corresponding increase in the probability P° with which the Li<sup>+</sup> ion will scatter as a neutral atom (ground state or otherwise). In this range of work function values, P<sup>-</sup> is

less than a few percent. However, as the work function further decreases, P<sup>-</sup> begins to increase at the expense of P°. For work function values less than about 2.6 eV, P<sup>+</sup> is less than a few percent.

In addition to the overall charge state fractions presented above, we have determined the relative yield of Li<sup>+</sup> ions scattered into the Li(2p) state by measuring the rate at which photons corresponding to the Li(2p)  $\longrightarrow$  Li(2s) transition ( $\lambda$ =673 nm) are produced. <sup>11-14</sup> A plot of the relative yield is shown in figure 2 for 400eV incident Li<sup>+</sup> (open circles). (The absolute yields of the Li(2p) states are estimated to be less than 1%.) When the surface is clean, we observe no photons to within the sensitivity of our detector. However, as the work function decreases, the photon yield increases, reaches a peak value, and then decreases. The distinctive feature of these data is the peak in the yield at a work function shift of about -1.8 eV. Also shown in figure 2 is the photon yield for 100eV incident Li<sup>+</sup> (open triangles), which also shows a peak in the photon yield as a function of decreasing work function. When the energy is decreased from 400eV to 100eV, the photon yield decreases by about an order of magnitude and shifts to lower work function shifts. A similar peak has been observed when 1 keV Li<sup>+</sup> was scattered at grazing angles from Cs/W(110). <sup>15,16</sup>

# Modeling:

To model these experiments we require a charge transfer calculation which can treat the simultaneous interactions of several atomic resonances with the surface electronic states. Such a many body calculation must include excited atomic states and affinity levels. Brad Marston (at Brown University) has developed such a code. His calculation employs a 1/n expansion (equivalent to a variational expansion of the many-body wavefunction in particle-hole pairs) to study the dynamics of charge-transfer involving degenerate orbitals. This expansion has been employed with success in the Kondo problem, and by Brako and Newns who earlier applied it to the charge transfer problem.<sup>17</sup> Marston has extended their treatment by including level crossings, excited atomic states and affinity levels. Input to the model includes the energies and lifetimes of the atomic resonances outside the surface. Details of the calculations are given elsewhere.<sup>14</sup>

#### Discussion:

In figure 1 the solid curves represent charge state fractions calculated using Marston's multiple-states model. Energies and lifetimes of the Li atomic states were taken from calculations by Nordlander and Tully (we have also used Li<sup>-</sup> lifetimes calculated by Gauyacq and Teillet-Billy). Shown in figure 2 are the calculated Li(2p) yields. The two curves in figure 2 are for 400eV and 100eV Li scattering. The calculated curve for 400eV has been normalized to the data.

The model reproduces the absolute yields of positive and negative ions, and qualitatively reproduces the peak in the photon yield, the decrease in the photon yield as the ion energy is decreased from 400eV to 100eV, and the shift in the peak that occurs when the beam energy decreases from 400eV to 100 eV. Note that the calculated peaks in figure 2 are narrower than the experimental ones; we believe that this is a result of adsorbate-induced inhomogeneities in the surface electrostatic potential caused by the alkali adsorbates, which is not included in the calculation.

Given the agreement between the measured and calculated yields, we can now use the model to extract information about the dynamics of the charge transfer process. A detailed analysis is quite lengthy<sup>20</sup> and will not be given here. Rather, key results are summarized below.

- 1. The charge state yields, i.e., yields of Li<sup>+</sup> and Li<sup>-</sup> (see figure 1), can be understood by considering the relative energies of the Fermi level and the Li(2s) (ionization) and Li(2s<sup>2</sup>) (affinity) levels. The Fermi level of clean Cu(001) lies 4.59eV below the vacuum level. For a Li atom far from the surface, the Li(2s) level lies 5.4eV below the vacuum level, while the Li(2s<sup>2</sup>) lies 0.62eV below the vacuum. For scattering from the clean surface, the adiabatic ground state is for the Li to scatter as a neutral. However, due to the finite velocity of the scattered particles and the shift in energy of the Li(2s) level near the surface, a significant Li<sup>+</sup> yield is observed in the scattered flux. As the work function decreases (by adsorbing Cs onto the Cu surface), the Li(2s) level lies further below the Fermi level, and more neutralization occurs. This trend continues until essentially no Li<sup>+</sup> is observed in the scattered flux. At very low work functions, it becomes energetically possible to fill the Li(2s<sup>2</sup>) level, which results in scattering of Li<sup>-</sup>. The Li<sup>-</sup> yield increases with decreasing work function.
- 2. The Li(2p) (see figure 2), in particular the <u>peak</u> versus  $\Delta\Phi$ , requires a more complicated explanation. Since the Li(2p) level lies 3.54eV below the vacuum, from energetic considerations, it is not expected to form in Li scattering from clean Cu(001). As the work function decreases, the Li(2p) yield increases as expected. Based simply on energetic considerations, one would expect the Li(2p) yield to increase monotonically with decreasing work function. However, both the experiment and calculations give a <u>peak</u> in the Li(2p) yield with decreasing work function.

The existence of the peak in the Li(2p) yield is a manifestation of many-body effects in the charge transfer. At the lowest work functions (i.e., largest  $\Delta\Phi$ ), a "competition" develops between the Li(2p) and Li states; thus the increase in the formation of negative ions results in a decrease in the negative ion yield. A more detailed analysis of the model indicates that there are additional interactions of the Li(2p) state with Li states other than the affinity level.  $^{20}$ 

The dynamics of the formation of the excited Li(2p) state are complex. However, the following key conclusions can be drawn:

- a. The finite velocity of the scattered particle is essential for the formation of scattered Li(2p); the Li(2p) is an excited state of the system, and will only form nonadiabatically because of the finite velocity of the scattered particles. Note that the Li(2p) yield decreases as the Li energy decreases from 400eV to 100eV,i.e., the system becomes more adiabatic with decreasing energy.
- b. The relative energies of the atomic state and the Fermi level are important in the formation of the Li(2p) peak. Significant population of the Li(2p) level cannot occur until the work function decreases significantly from its clean surface value.
- c. Whether the Li(2p) survives in the scattered flux will also depend on competition with other states, such as the Li<sup>-</sup> state.

We have also made preliminary measurements of the formation of Na(3p) (excited state neutrals) in the scattering of 400eV Na<sup>+</sup> from Cs-covered Cu(001). A peak in the

yield of Na(3p) versus  $\Delta\Phi$  is observed. These results, as well as the corresponding multistate calculation, are shown in figure 3. As expected from the discussion above, since the Na(3p) level is higher in energy than the Li(2p) level (by about 0.5 eV) the peak in the Na(3p) yield is shifted to lower work functions (larger  $\Delta\Phi$ ). We are in the process of making more careful measurements of the Na(3p) yields.

A new monochromator system has been developed in our lab; we are currently using it to search for the formation of higher-lying excited states of scattered Li.

# Trajectory-dependent charge transfer for Na<sup>+</sup> scattering from Cu(001)

# Motivation:

We have observed trajectory-dependent charge transfer in Na<sup>+</sup> scattering from Cu(001).<sup>21</sup> To our knowledge, this is the first report of trajectory-dependent charge transfer in alkali scattering from clean (i.e., adsorbate-free) metal surfaces. In scattering of 7.5eV and 50eV Na<sup>+</sup> from Cu(001), we have measured neutralization probabilities ranging from 0.07 to 0.5 for two Na trajectories leaving the surface with the same speed and direction, but with different collisional histories. This is in contrast to earlier work showing that, for the Na/Cu system in the same velocity range, the neutralization scales with final perpendicular velocity, and is independent of collision history.<sup>6</sup> Modeling indicates that the different surface atomic displacements produced in the different types of collisions can explain the dramatic variation in neutralization with collision type.

# **Experiments:**

A 50 eV mass-selected, monoenergetic beam of Na<sup>+</sup> was scattered from Cu(001) along the  $\langle 100 \rangle$  azimuth. Figure 4 shows a time-of-flight spectrum for the scattered particles for  $\theta_i = 30^\circ$  and  $\theta_f = 35^\circ$ , both measured from the surface normal. The Cu(001) crystal was held at a temperature of 160 K during these measurements to reduce surface atom thermal motions. The scattered particle intensity is plotted as a function of the normal component of the scattering velocity  $v_{\perp}$  in atomic units (1 au=2.2×10<sup>8</sup> cm/s). The dotted curve in figure 4 shows the scattered ions, while the solid curve shows the scattered neutrals. The open circles show the neutral fraction, obtained by taking the ratio of scattered neutral flux to the total flux (ions plus neutrals). Figure 5 shows similar measurements (i.e., same scattering geometry and surface temperature) for 7.5 eV incident Na<sup>+</sup>.

In figure 4, the neutral fraction over most of the scattered velocities  $(v_{\perp} > .003)$  is on the order of a few percent. The neutral fraction for the lowest velocity peak (centered on  $v_{\perp} \approx .002$ ) in figure 5 is on the order of 0.5. In contrast to this, in figure 5 the neutral fraction for the peak centered on  $v_{\perp} \approx .002$  is on the order of .1 to .2. This is a somewhat surprising result since previous charge transfer experiments on the Na/Cu system, as well as charge transfer models, predict that the neutralization probability will depend on the velocity of the scattered particle. Note that the two peaks in figures 4 and 5, both centered on  $v_{\perp} \approx .002$ , have almost identical outgoing velocities and angles.

#### Modeling:

In this discussion we will focus primarily on the two peaks in figures 4 and 5 that are centered on  $v_{\perp} \approx .002$ . Due to the difference in incident energies, i.e., 50eV and 7.5eV, respectively, these peaks correspond to different types of scattering trajectories. A

detailed analysis of these trajectory types can be obtained using our classical trajectory code SAFARI, with scattered potentials that have been shown to work over a wide energy range.<sup>22-25</sup>

In figure 4, the lowest velocity peak, centered on  $v_{\perp} \approx .002$  au, corresponds to collisions involving first and second layer atoms, such as those shown in figures 3e and 3f. Trajectory 3f is the dominant trajectory type in the peak. The particles in this peak have final energies on the order of 3 eV, after having transferred approximately 47 eV to a few surface atoms.

Trajectory analysis of the spectra in figure 5 indicates that the peak centered on  $v_{\perp} \approx .002$  au is dominated by quasi-double collisions with top-layer surface atoms (i.e., there is no penetration of the top layer). The scattered particles have approximately 3 eV of energy, having transferred  $\sim 4$  eV to two top-layer surface atoms.

In figure 1, the intensity peak between .004  $< v_{\perp} <$  .006 corresponds to Na scattering from the top layer of the Cu(001) crystal; they include quasi-single and quasi-double collisions involving momentum transfer to primarily one or two surface atoms, respectively, along top layer  $\langle 100 \rangle$  chains of atoms. Also included are "zig-zag" collisions involving top layer collisions with atoms on adjacent  $\langle 100 \rangle$  chains. Side and top views of these trajectories are shown in figures 3a-3d.

# Discussion:

As mentioned above, the unexpected result found in these studies is that the two peaks centered at  $v_{\perp} \sim .002$  au in figures 4 and 5 differ significantly in neutralization probability, yet they correspond to nearly identical exit trajectories (i.e., same final velocities and angles). According to widely accepted theories of alkali ion-metal scattering, one expects the charge transfer to depend only on the outgoing trajectory. This expectation arises from the following considerations: at the distance of closest-approach the Na atomic levels are strongly hybridized with the surface electronic states. Thus their lifetimes are short compared to the timescale of the atomic motion, and the Na atoms are in electronic equilibrium with the surface, independent of the incident trajectory or charge state. The final charge state of the scattered Na is then determined on the outgoing trajectory. For a Na leaving an unperturbed surface, which we typically assume to be the case, one would expect neutral fractions on the order of a few percent at the velocities we use in these experiments.

Why then do we observe neutral fractions of 0.5 for the low velocity peak in figure 4? We believe the explanation lies in the coupling of the charge transfer and collision dynamics. Recall that this peak is dominated by second layer scattering trajectories, similar to that shown in figure 3f, in which there has been a large energy transfer to a small number of surface atoms. This energy transfer can result in atoms recoiling from their lattice sites, creating lattice defects; the Na leaves the surface through a perturbed region created by the collision itself. Thus the surface can no longer be modeled as a perfect Cu(001) crystal, but as one that has an atomic scale defect in the vicinity of the departing Na particle. Associated with this defect will be a perturbed local electrostatic potential, which can be approximated by an electrostatic dipole, similar to that around an adsorbed atom on the surface. This dipole locally mimics a work function decrease, which results in increased neutralization. Using a model of the single-electron charge transfer process, we have estimated that a dipole moment on the order of .75D is required to

give the observed neutralization. This is consistent with dipole moments that have been estimated for atomic-scale surface defects from other types of measurements.<sup>26</sup>

In summary, we believe that we have demonstrated, for the first time, a coupling of the charge transfer and collision dynamics for alkali scattering from a clean metal surface.

# Future work:

In ongoing and future work, we will continue our studies of multi-channel charge transfer dynamics. This includes the above-mentioned measurements of the excited state formation of Na(3p) and the higher-lying excited states of Li. We also plan to continue our studies of charge transfer in oxygen scattering. The collaboration with Marston in interpreting these results will continue.

As stated in the introduction to this report, our goal is to incorporate our understanding of charge transfer processes into an integrated picture of the dynamics of hyperthermal ion scattering from surfaces. Clearly the ion-surface scattering potential is a function of the charge state of the incident ion. One obvious feature of the alkali-metal potential is the attractive interaction close to the surface due to the induced image charge in the metal. The neutral species will not induce an image charge. At low incident energies, this induced image charge has a dramatic effect on the scattered energies and angles, the energy transferred to the surface, and the trapping of the scattered particle in the attractive ion-surface potential well.<sup>23</sup> We are beginning experimental studies of trapping and embedding behavior in hyperthermal ion-surface collisions. The initial trapping measurements will be made for Na<sup>+</sup> and O<sup>+</sup> incident on clean Cu(001). These two species are similar in mass, thus we expect their scattering dynamics to be similar. However, they have very different charge transfer behavior and scattering potentials, which may dramatically influence their trapping probabilities.

#### IV. REFERENCES

- <sup>1</sup>P.W. Amersfoort, J.J.C. Geerlings, L.F.Tz. Kwakman, E.H.A. Granneman, and J. Los, J. Appl. Phys. 58, 2312 (1985).
  - <sup>2</sup>G.A. Kimmel and B.H. Cooper, Rev. Sci. Instrum. 64, 672 (1993).
  - <sup>3</sup>P. Nordlander and J.C. Tully, Surf. Sci. **211/212**, 207 (1989).
  - <sup>4</sup>D. Teillet-Billy and J.P. Gauyacq, Surf. Sci. 239, 343 (1990).
  - <sup>5</sup>J.P. Gauyacq and D. Teillet-Billy, submitted for publication.
  - <sup>6</sup>G.A. Kimmel and B.H. Cooper, Phys. Rev. B 48, 12164 (1993).
  - <sup>7</sup>S. Schubert, U. Imke, and W. Heiland, Surf. Sci. 219, L576 (1989).
- <sup>8</sup>S. Schubert, U. Imke, W. Heiland, K.J. Snowdon, P.H.F. Reihnen, and A.W. Kleyn, Surf. Sci. 205, L793 (1988).
  - <sup>9</sup>R. Brako and D.M. Newns, Rep. Prog. Phys. **52**, 655 (1989).
  - <sup>10</sup>R. Brako and D.M. Newns, Surf. Sci. 108 253 (1981).
- <sup>11</sup>B.H. Cooper and E.R. Behringer, in Low Energy Ion-Surface Interactions, Advances in Ion Chemistry and Physics, J. Wayne Rabalais (ed.), John Wiley & Sons, Ltd: Sussex,

1994.

- <sup>12</sup>E.R. Behringer, D.R. Andersson, D.M. Goodstein, B.H. Kasemo, B.H. Cooper and J.B. Marston, Nucl. Instrum. and Meth. in Phys. Res. B, 78, 3 (1993).
- <sup>13</sup>D.R. Andersson, E.R. Behringer, B.H. Cooper and J.B. Marston, J. Vac. Sci. Technol., A11, 2133 (1993).
- <sup>14</sup>J.B. Marston, D.R. Andersson, E.R. Behringer, B.H. Cooper, C.A. DiRubio, G.A. Kimmel and C. Richardson, Phys. Rev. B 48, 7809 (1993).
- <sup>15</sup>H. Schall, W. Huber, H. Hoermann, W. Maus-Friedrichs, and V. Kempter, Surf. Sci. **210**, 163 (1989).
  - <sup>16</sup>H. Schall, H. Brenten, K.H. Knorr and V. Kempter, Z. Phys. D16, 161 (1990).
  - <sup>17</sup>R. Brako and D.M. Newns, Solid State Comm. **55** 633 (1985).
  - <sup>18</sup>P. Nordlander, private communication.
  - <sup>19</sup>J.P. Gauyacq and D. Teillet-Billy, private communication.
  - <sup>20</sup>E.R. Behringer, D.R. Andersson, B.H. Cooper and J.B. Marston, in preparation.
  - <sup>21</sup>C.A. Keller, C.A. DiRubio, G.A. Kimmel and B.H. Cooper, in preparation.
- <sup>22</sup>B.H. Cooper, C.A. DiRubio, G.A. Kimmel and R.L. McEachern, Nucl. Instrum. and Meth. Bo4, 49 (1992).
  - <sup>23</sup>C.A. DiRubio, R.L. McEachern, J.G. McLean, and P.H. Cooper, in preparation.
  - <sup>24</sup>D.L. Adler and B.H. Cooper, Phys. Rev. B43, 3876 (1991).
  - <sup>25</sup>D.M. Goodstein, R.L. McEachern, and B.H. Cooper, Phys. Rev. B 39, 13129 (1989).
  - <sup>26</sup>K. Besocke and H. Wagner, Phys. Rev. B 8, 4957 (1973).

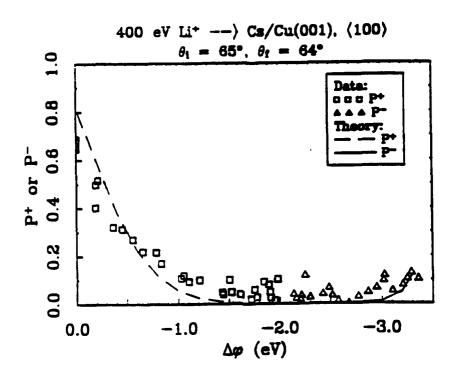


Figure 1: Measured and calculated values of the positive and negative charge state fractions for scattered Li versus the work function shift  $\Delta\Phi$  induced by cesium adsorbates. Li<sup>+</sup> ions with an incident energy of 400eV impinge on a Cu(001) surface along the (100) azimuth with an incident angle of  $\theta_i = 65^{\circ}$  measured with respect to the surface normal. Particles scattered into  $\theta_f = 64^{\circ}$  are detected.  $\Delta\Phi$ =0.0 corresponds to the clean surface with  $\Phi$ =4.59eV. The calculated charge state fractions were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully.

Normalized Intensity of Li(2p-2s) emission vs.  $\Delta \varphi$ 100 & 400eV Li+ --> Cs/Cu(001) along  $\langle 100 \rangle$ ,  $\theta_i = 65^{\circ}$ Normalized Intensity 400eV Li+ 100eV Lit 400eV Li+ 0 9 0 80 ō8 99 8 0 <sub>9</sub> 00 0 -3.0 -2.0 -1.0 0.0  $\Delta \varphi$  (eV)

Figure 2: Measured and calculated values of the relative yield of excited neutral atoms in the Li(2p) state versus the work function shift  $\Delta\Phi$  induced by cesium adsorbates. Li<sup>+</sup> ions with incident energies of 400eV and 100 eV impinge on a Cu(001) surface along the (100) asimuth with an indicent angle of  $\theta_i = 65^{\circ}$  measured with respect to the surface normal. Photons corresponding to the Li(2p)—Li(2s) transition ( $\lambda = 673$ nm) are detected. The calculated values were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully. The calculated curve with the larger magnitude corresponds to 400eV scattering, and is normalized to the data.

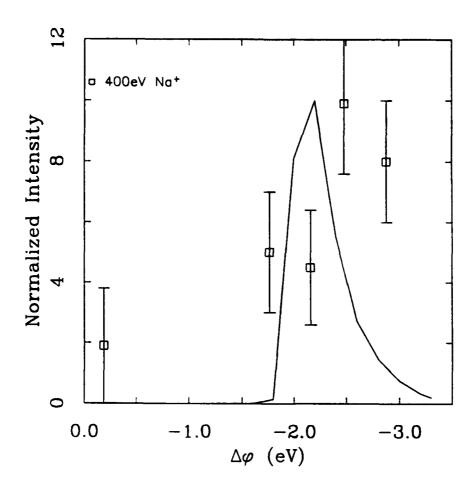


Figure 3: Measured and calculated values of the relative yield of excited neutral atoms in the Na(3p) state versus the work function shift  $\Delta\Phi$  induced by cesium adsorbates. Na<sup>+</sup> ions with incident energies of 400eV impinge on a Cu(001) surface along the (100) azimuth with an indicent angle of  $\theta_i = 65^{\circ}$  measured with respect to the surface normal. Photons corresponding to the Na(3p)—Na(3s) transition ( $\lambda = 589$ nm) are detected. The calculated values were obtained using Marston's multi-state charge transfer model with alkali state energies and lifetimes from Nordlander and Tully. The calculated curve is normalized to the data.

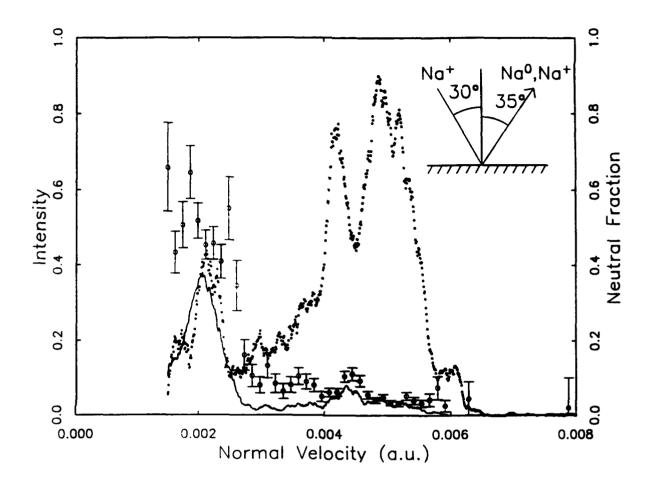


Figure 4: Neutral (solid curve) and ion (dotted curve) spectra for 50eV Na<sup>+</sup> scattered from Cu(001) along the (100) azimuth, with  $\theta_i = 30^{\circ}$  and  $\theta_f = 35^{\circ}$ . Also shown (circles with statistical error bars) is the neutralisation probability versus perpendicular velocity of the scattered particles. The velocity is given in atomic units; 1 au= $2.2 \times 10^8$ cm/s. Note the much larger neutralisation probability for the low velocity peak.

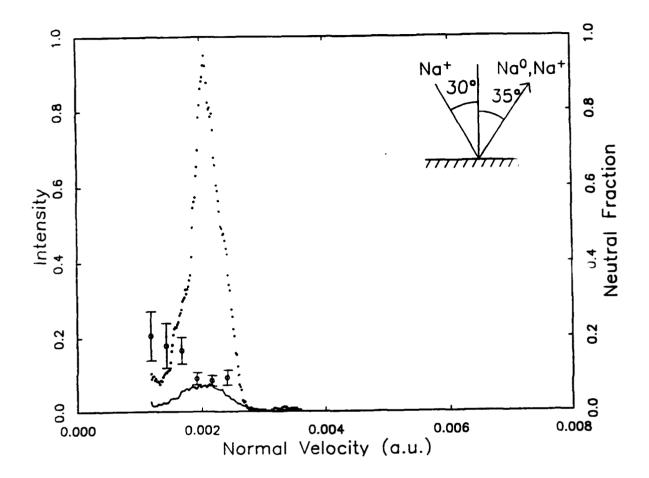


Figure 5: Neutral (solid curve) and ion (dotted curve) spectra for 7.5eV Na<sup>+</sup> scattered from Cu(001) along the  $\langle 100 \rangle$  azimuth, with  $\theta_i = 30^\circ$  and  $\theta_f = 35^\circ$ . Also shown (circles with statistical error bars) is the neutralization probability versus perpendicular velocity of the scattered particles. At the same final velocity, this set of spectra shows a much smaller neutralization probability than the low velocity peak in figure 4.

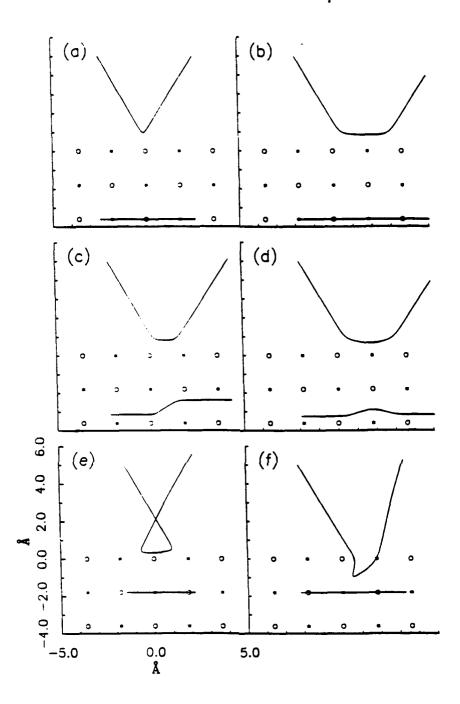


Figure 6: Scattering trajectories for 50eV Na<sup>+</sup> scattered from Cu(001) along the  $\langle 100 \rangle$  azimuth, with  $\theta_i = 30^\circ$  and  $\theta_f = 35^\circ$ . In each panel the upper curve is a side view of the trajectory, while the lower curve is a top-down view looking directly into the crystal surface. The open circles represent foreground atoms while the asterisks represent the next layer atoms.

# VI. RESEARCH PARTICIPANTS

Participants in the charge exchange research program include B.H. Cooper (partial summer salary from AFOSR-91-0137) and graduate students G.A. Kimmel, D.R. Peale, S.T. Tsao, and C. Wengel and postdoctoral fellow D. Goodstein (supported by AFOSR-91-0137). Graduate students E. Behringer (supported by MSC-NSF-DMR-8516616) and C. Keller (supported by a Hertz Fellowship), and postodtoral fellow D. Andersson (supported by the Sweden-America Foundation and NSF) are also working on charge transfer. Also working on the apparatus and involved in related research programs are graduate students J. McLean (supported by AASERT) and E. Dahl (supported by an AT&T Fellowship). Brad Marston from Brown University is collaborating with us on theoretical modeling of charge transfer processes.

# VII. PUBLICATIONS

- 1) "The Design and Performance of a UHV Beamline to Produce Low and Hyperthermal Energy Ion Beams," D.L. Adler and B.H. Cooper, Rev. Sci. Instrum. 59, 137 (1988).
- 2) "An Efficient Algorithm for the Simulation of Hyperthermal Energy Ion Scattering," D.M. Goodstein, S.A. Langer, and B.H. Cooper, J. Vac. Sci. Technol. A 6, 703 (1988), AVS conference proceedings.
- 3) "Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion Scattering, D.L. Adler, B.H. Cooper, and D.R. Peale, J. Vac. Sci. Technol. A 6, 804 (1988), AVS conference proceedings.
- 4) "A Versatile Apparatus for Low Energy and Hyperthermal Energy Ion Scattering Spectroscopy," R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, B.R. Litt, D.R. Peale, and B.H. Cooper, Rev. Sci. Instrum. 59, 2560 (1988).
- 5) "Trajectory Analysis of Low Energy and Hyperthermal Ions Scattered from Cu(110)," R.L. McEachern, D.M. Goodstein, and B.H. Cooper, Phys. Rev. B 39, 10503 (1989).
- 6) "Low Energy Alkali Ion Scattering as a Probe of Resonant Charge Exchange on Cesiated Cu (110)," G.A. Kimmel, D.M. Goodstein, and B.H. Cooper, J. Vac. Sci. Technol. A7, 2186 (1989), 1988 AVS conference proceedings.
- 7) "Ion-Surface Interaction Potentials from Alkali-Ion-Metal Scattering Below 500 eV," D.M. Goodstein, R.L. McEachern, and B.H. Cooper, Phys. Rev. B 39, 13129 (1989).
- 8) "A Source for Producing Alkali Ion Beams for Low-Energy Surface Scattering Spectroscopies," D.L. Adler, B.R. Litt, D.R. Peale, and B.H. Cooper, Rev. Sci. Instrum. 60, 730 (1989).
- 9) "A Scanning Tunneling Microscope for UHV Atom-Surface Interaction Studies," D.R. Peale and B.H. Cooper, J. Vac. Sci. Technol. A8, 345 (1990).
- 10) "Energy and Angular Distributions of 100 eV to 400 eV Na<sup>+</sup> Scattered from Cu(110)," D.L. Adler and B.H. Cooper, Phys. Rev. B 43, 3876 (1991).

- 11) "Local Adsorbate-Induced Effects on Dynamical Charge Transfer in Ion-Surface Interactions," G.A. Kimmel, D.M. Goodstein, Z.H. Levine, and B.H. Cooper, Phys. Rev. B 43, 9403 (1991).
- 12) "Low Energy Ion-Surface Interactions," B.H. Cooper, C.A. DiRubio, G.A. Kimmel, and R.L. McEachern, Nucl. Instr. and Meth. in Phys. Res. B64, 49 (1992).
- 13) "Adsorbate-Promoted Mass Flow on the Gold(111) Surface Observed by Scanning Tunneling Microscopy," D.R. Peale and B.H. Cooper, J. Vac. Sci. Technol. A 10, 2210 (1992).
- 14) "A Time-of-Flight Spectrometer for Low Energy Neutral and Ionized Alkalis," G.A. Kimmel and B.H. Cooper, Rev. Sci. Instrum. 64, 672 (1993).
- 15) "Charge Transfer Dynamics of Low Energy Collisions of Li<sup>+</sup> with Alkali-covered Cu(001)," E.R. Behringer, D.R. Andersson, D.M. Goodstein, B.H. Kasemo, B.H. Cooper, and J.B. Marston, Nucl. Instr. and Meth. in Phys. Res. B 78, 3 (1993).
- 16) "Excited State Formation in Low Energy Li<sup>+</sup>-Surface Collisions," D.R. Andersson, E.R. Behringer, B.H. Cooper, and J.B. Marston, J. Vac. Sci. Technol. A11, 2133 (1993).
- 17) "Mass Flow and Stability of Nanoscale Features on Au(111)," B.H. Cooper, D.R. Peale, J.G. McLean, R. Phillips, and E. Chason, in *Evolution of Surface and Thin Film Microstructure*, eds. H.A. Atwater, E. Chason, M.H. Grabow, and M. Lagally, MRS Symposia Proc. Vol. 280 (MRS, Pittsburgh, PA), 1993.
- 18) "Surface Diffusion: Atomistics and Surface Morphology," M.H. Grabow, P.J. Feibelman, G.H. Gilmer, B.H. Cooper, and Y.W. Mo, in *Evolution of Surface and Thin Film Microstructure*, eds. H.A. Atwater, E. Chason, M.H. Grabow, and M. Lagally, MRS Symposia Proc. Vol. 280 (MRS, Pittsburgh, PA), 1993.
- 19) "Many-Body Theory of Charge Transfer in Hyperthermal Atomic Scattering," J.B. Marston, D.R. Andersson, E.R. Behringer, B.H. Cooper, C.A. DiRubio, G.A. Kimmel, and C. Richardson, Phys. Rev. B 48, 7809 (1993).
- 20) "The Dynamics of Resonant Charge Transfer in Low Energy Alkali Ion Scattering," G.A. Kimmel and B.H. Cooper, Phys. Rev. B 48, 12164 (1993).
- 21) "The Dynamics of Hyperthermal Na<sup>+</sup> Scattering from Cu(001): The Role of the Attractive Interaction," C.A. DiRubio, R.L. McEachern, J.G. McLean, and B.H. Cooper, in preparation.
- 22) "Quantitative Detection of Low Energy Positive and Negative Ions With a Channel Electron Multiplier," C.A. Keller and B.H. Cooper, in preparation.
- 23) "Charge Transfer in Low Energy Scattering of O<sup>+</sup> from Cu(001)," C.A. Keller and B.H. Cooper, in preparation.
- 24) "Multi-Channel Charge Transfer in Li Scattering from Alkali-Covered Cu(001)," E.R. Behringer, D.R. Andersson, B.H. Cooper and J.B. Marston, in preparation.

- 25) "Limitations of the Trajectory Approximation in Atom-Surface Scattering," C.A. Dirubio, B.H. Cooper and K. Burke, submitted for publication.
- 26) "The Influence of Surface Dynamics on Hyperthermal Energy Ion-Surface Collisions," C.A. DiRubio, B.H. Cooper and K. Burke, in preparation.
- 27) "Probing Surface Lattice Dynamics with Hyperthermal Ion Scattering," D.M. Goodstein, C.A. DiRubio, B.H. Cooper, and K. Burke, submitted to Surface Reviews and Letters.
- 28) "Energy and Angular Distributions of 100 and 400 eV Li Scattering from Cu(001)," E.R. Behringer, J.G. McLean, and B.H. Cooper, in preparation.
- 29) "Mass Flow from Nonequilibrium Nano-Structures on the Au(111) Surface Observed by Scanning Tunneling Microscopy," D.R. Peale, J.G. McLean, R. Phillips, E. Chason, and B.H. Cooper, in preparation.
- 30) "Trajectory-Dependent Charge Transfer in Hyperthermal Energy Scattering of Na+from Cu(001)," C.A. Keller, C.A. DiRubio, and B.H. Cooper, in preparation.

# BOOK CHAPTER

31) "Scattering and Charge Transfer Dynamics in Low and Hyperthermal Energy Alkali Ion-Surface Collisions," in Low Energy Ion-Surface Interactions, Advances in Ion Chemistry and Physics, J. Wayne Rabalais (ed.), John Wiley & Sons, Ltd: Sussex, 1994.

#### OTHER ARTICLES

- 32) "Fundamentals of Ion-Surface Interactions: Techniques for Efficient Simulations of Hyperthermal Energy Ion Scattering," B.H. Cooper, D.M. Goodstein, and S.A. Langer, Forefronts, published by the Center for Theory and Simulation in Science and Engineering, Cornell University (January 1988).
- 33) "Interactions of Hyperthermal Ions at Metal Surfaces," B.H. Cooper, D.M. Goodstein, G.A. Kimmel, R.L. McEachern, proceedings of the Third Annual Workshop on Surface Reactions in the Space Environment, Vanderbilt University (1988).
- 34) "Effects of Surface Adsorbates on Resonant Electron Transfer," B.H. Cooper, D.M. Goodstein, and G.A. Kimmel, proceedings of the Fourth Annual Workshop on Surface Reactions in the Space Environment, Northwestern University (1989).
- 35) "Scattering Potentials for Ion-Surface Collisions in the 10-200 eV Range," proceedings of the Fifth Annual Workshop on Surface Reactions in the Space Environment, Northwestern University (1990).
- 36) "Charge Transfer and Trapping Dynamics in Hyperthermal Ion-Surface Collisions," B.H. Cooper, C.A. DiRubio, G.A. Kimmel, and C.A. Keller, submitted to Proceedings of the Sixth Annual Workshop on Surface Reactions in the Space Environment,

Northwestern University (1991).

- 37) "Mass Flow and Stability of Nanoscale Features on Au(111): The Role of Adsorbates," D.R. Peale, J.G. McLean, and B.H. Cooper, extended abstracts from the DOE Workshop on Surface Diffusion and Growth of Materials, Sante Fe, NM (1992).
- 38) "Probing the Dynamics of Hyperthermal Energy Atom-Surface Interactions with Charge-State Resolved Scattering Measurements," D.R. Andersson, E.R. Behringer, C. Keller, C.A. DiRubio, G. Kimmel, B.H. Cooper, and J.B. Marston, Proceedings of the Seventh Annual Workshop on Surface Reactions in the Space Environment, Skokie, IL (1992).

# **GROUP THESES**

"Design, Construction and Characterization of a Low Energy Alkali Ion Source," Barbara R. Litt, Cornell Physics Masters Thesis (1986).

"Kinematics of Hyperthermal Energy Ion Scattering," David L. Adler, Cornell Physics Ph.D. Thesis (1989).

"Trajectory and Impact Parameter Analysis of Hyperthermal Ion Scattering," Randall L. McEachern, Cornell Physics Ph.D. Thesis (1990).

"Energy and Charge Transfer in Hyperthermal Ion-Surface Scattering," David M. Goodstein, Cornell University Ph.D. Thesis (1990).

"Diffusion and Mass Flow Dynamics on the Gold(111) Surface Observed by Scanning Tunneling Microscopy," David Reese Peale, Cornell Physics Ph.D. Thesis (1992).

"The Dynamics of Resonant Charge Exchange in Low Energy Ion-Surface Interactions," Gregory Allen Kimmel, Cornell Physics Ph.D. Thesis (1992).

"The Dynamics of Energy Transfer in Hyperthermal Energy Ion Scattering from Metal Surfaces," Christopher Auguste DiRubio, Cornell Physics Ph.D. Thesis (1993).

"The Dynamics of Resonant Charge Transfer in Hyperthermal Energy Ion-Surface Collisions," Ernest Robert Behringer, Cornell Physics Ph.D. Thesis (1994).

#### VIII. PRESENTATIONS

- 1) Computer Simulations of Hyperthermal Ion Scattering: Measuring Short-Range Surface Order in Crystals,
  - B.H. Cooper and D.M. Goodstein, presented at the Sixth International Workshop on Inelastic Ion Surface Collisions, Argonne National Laboratory, August 1986. (poster presentation)
- 2) Hyperthermal Ion-Surface Scattering Simulation: Alternatives to Monte Carlo, D.M. Goodstein, S.A. Langer, and B.H. Cooper, presented at the New York Meeting of the American Physical Society, March 1987. (poster presentation)

- 3) A Versatile Apparatus for Low Energy and Hyperthermal Ion Scattering, R.L. McEachern and B.H. Cooper, presented at the New York meeting of the American Physical Society, March 1987. (oral presentation)
- 4) An Ion Scattering System for the Energy Range 10 eV to 10 keV,
  D.L. Adler and B.H. Cooper, presented at the New York meeting of the American
  Physical Society, March 1987. (oral presentation)
- 5) Ion-Surface Scattering at Low and Hyperthermal Energies: Scattering Dynamics and Charge Exchange in Relation to Surface Chemistry,

  B.H. Cooper, invited talk at the American Chemical Society Meeting, New Orleans, September 1987.
- 6) Ion Surface Scattering at Hyperthermal Energies: Scattering Dynamics and Charge Exchange,
  - B.H. Cooper, talk at the AFOSR Surface Chemistry Contractor's Conference, Colorado Springs, September 1987.
- 7) Interactions of Hyperthermal Ion Beams with Metal Surfaces, D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the 34<sup>th</sup> National Symposium of the American Vacuum Society, Anaheim, California, November 1987. (poster presentation)
- 8) Design and Performance of Ion Optics for Hyperthermal (10-100 eV) and keV Ion Scattering,
  - D.L. Adler, B.H. Cooper, and D.R. Peale, presented at the 34<sup>th</sup> National Symposium of the American Vacuum Society, Anaheim, California, November 1987. (poster presentation)
- 9) Scattering Dynamics of Low Energy Alkali and Noble Gas Ions Incident on Cu(110), R.L. McEachern, D.L. Adler, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
- 10) Low Energy Ion Scattering Studies of Surfaces Disordered by Ion Bombardment, G.A. Kimmel, D.L. Adler, D.M. Goodstein, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
- 11) Structural Study of the O/Cu(110) System Using Hyperthermal and Low Energy
  Noble Gas and Alkali Ion Scattering,

  D.L. Adler, R.L. McEachern, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper.
  - D.L. Adler, R.L. McEachern, D.M. Goodstein, G.A. Kimmel, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)
- 12) Hyperthermal Alkali Ion Scattering from Cu(110),

  D.M. Goodstein, D.L. Adler, R.L. McEachern, and B.H. Cooper, presented at the New Orleans meeting of the American Physical Society, March 1988. (oral presentation)

- 13) Low and Hyperthermal Energy Ion-Surface Scattering: Trajectory Analysis, Multiple Scattering, and Charge Exchange,
  - B.H. Cooper, invited talk at Rutgers University, Piscataway, NJ, April 1988.
- 14) Scattering of 50 eV to 4 keV Alkali Ion Beams from Cu(110) Surfaces: Trajectory Analysis and Charge Exchange,
  - B.H. Cooper, invited talk at Xerox Corporation, Webster, NY, June 1988.
- 15) Ion-Surface Scattering at Hyperthermal and keV Energies: Interaction Potentials,
  Trajectory Analysis, and Charge Exchange,

  B. H. Cooper, talk at the 48<sup>th</sup> Appeal Conference on Physical Electronics.
  - B.H. Cooper, talk at the 48<sup>th</sup> Annual Conference on Physical Electronics, Brookhaven Labs, June 1988.
- 16) Low Energy Ion Scattering as a Probe of Resonant Charge Exchange on Cu(110), G.A. Kimmel, R.L. McEachern, D.L. Adler, D.M. Goodstein, B.H. Cooper, presented at the 35<sup>th</sup> National Symposium of the American Vacuum Society, Atlanta, Georgia, October 1988. (oral presentation)
- 17) Hyperthermal Na<sup>+</sup> and K<sup>+</sup> Scattering as a Probe of Resonant Charge Exchange on Cu(110),
  - D.M. Goodstein, R.L. McEachern, B.H. Cooper, presented at the 35<sup>th</sup> National Symposium of the American Vacuum Society, Atlanta, Georgia, October 1988. (poster presentation)
- 18) Third Annual AFOSR Workshop on "Surface Reactions in a Space Environment", B.H. Cooper, invited talk, Vanderbilt University Center for Atomic and Molecular Physics at Surfaces, Nashville, TN, October 1988.
- 19) Alkali Ion-Surface Scattering at Hyperthermal Energies,
  B.H. Cooper, AFOSR Molecular Dynamics Contractors Conference, Newport
  Beach, CA, October 1988. (poster presentation)
- 20) Low Energy Ion Beam Scattering as a Probe of Ion-Surface Interactions, B.H. Cooper, invited talk, Michigan State University, Condensed Matter Physics Seminar, February 1989.
- 21) Ion-Surface Interactions at Hyperthermal Energies: Scattering and Charge Transfer Mechanisms,
  - B.H. Cooper, invited talk, presented at the St. Louis Meeting of the American Physical Society, March 1989.
- 22) Elastic and Inelastic Processes in Hyperthermal Ion-Surface Interactions,
  D.M. Goodstein, G.A. Kimmel, B.H. Cooper, B. Kasemo, presented at the St.
  Louis Meeting of the American Physical Society, March 1989. (oral presentation)
- 23) 100 to 400 eV Na<sup>+</sup> Scattering from Cu(110), D.L. Adler, D.M. Goodstein, and B.H. Cooper, presented at the St. Louis Meeting of the American Physical Society, March 1989. (oral presentation)
- 24) Low-Energy Ion Beam Scattering as a Probe of Ion-Surface Interactions,

- B.H. Cooper, invited talk, Molecular Beams Group of the Royal Society of Chemistry, Meeting on "Ions, Clusters, and Surfaces," Liverpool, England, April 1989.
- 25) Low and Hyperthermal Energy Ion Scattering Studies of Charge Transfer at Clean and Adsorbate-Covered Metal Surfaces,
  - B.H. Cooper, invited talk, Workshop on "Dynamics of Surface Reactions," Copenhagen, Denmark, May 1989.
- 26) A Vibration-Insensitive Thermally-Compensated Scanning Tunneling Microscopy for UHV Surface Studies,
  - D.R. Peale and B.H. Cooper, presented at the Scanning Tunneling Microscope Spring Workshop, University of Pennsylvania, Philadelphia, PA, May 1989. (poster presentation)
- 27) Hyperthermal Ion Scattering: Trajectory Analysis
  R.L. McEachern, Ph.D. job talk presented at AT&T Bell Laboratories, Murray
  Hill, NJ, April 1989; IBM Yorktown Heights, NY, April 1989; IBM Almaden,
  CA, May 1989; Sandia National Laboratories, Albuquerque, NM, May 1989.
- 28) A Scanning Tunneling Microscope for UHV Atom-Surface Interaction Studies,
  D.R. Peale and B.H. Cooper, presented at the 4<sup>th</sup> International Conference on
  Scanning Tunneling Microscopy, Oarai, Japan, July 1989. (poster presentation)
- 29) Hyperthermal Energy Ion Scattering as a probe of Charge Transfer at Surfaces, B.H. Cooper, invited talk, Gordon Conference on "Dynamics of Gas-Surface Interactions," Proctor Academy, Andover, NH, August 1989.
- 30) The Influence of Adsorbate-Induced Local Electronic Structure on Charge Exchange Processes at Surfaces,
  - G.A. Kimmel, D.M. Goodstein, B. Kasemo, and B.H. Cooper, presented at the Gordon Conference on "Dynamics of Gas-Surface Interactions," Proctor Academy, Andover, NH, August 1989. (poster presentation)
- 31) 10-100 eV Ion-Surface Interactions: Measurements and Classical Trajectory Simulations,
  - B.H. Cooper, invited talk, AFOSR Fourth Annual Workshop on Surface Reactions in the Space Environment, Northwestern University, September 1989.
- 32) The Influence of Local Electronic Structure on the Neutralization of Alkali Ions Scattered form Adsorbate-Covered Cu(001),
  - G.A. Kimmel, D.M. Goodstein, B. Kasemo, and B.H. Cooper, presented at the 36<sup>th</sup> National Symposium of the American Vacuum Society, Boston, MA, October 1989. (poster presentation)
- 33) Hyperthermal Energy Ion Scattering from the  $(2 \times 1)$  Oxygen Reconstructed Surface of Cu(110),
  - D.L. Adler, D.M. Goodstein, and B.H. Cooper, presented at the 36<sup>th</sup> National Symposium of the American Vacuum Society, Boston, MA, October 1989. (oral presentation)

- 34) A Scanning Tunneling Microscope for UHV Surface Studies, D.R. Peale and B.H. Cooper, presented at the Cornell National Nanofabrication Facility, 11<sup>th</sup> Annual Industrial Affiliates Meeting, October 1989. (oral presentation)
- 35) Local Adsorbate-Induced Effects on Non-Adiabatic Charge Transfer to Hyperthermal Energy Ions,
  - B.H. Cooper, talk at the AFOSR Molecular Dynamics Contractors Conference, Captiva Island, Florida, October 1989.
- 36) Energy, Momentum, and Charge Transfer in Hyperthermal Ion-Surface Interactions, D.M. Goodstein, Ph.D. job talk presented at University of Washington, Dept. of Chemistry, June 1989; AT&T Bell Laboratories, Holmdel, NJ, September 1989; IBM Yorktown Heights, NY, October 1989.
- 37) Dynamical Charge Transfer in Ion-Surface Interactions,
  B.H. Cooper, invited talk, Physical Chemistry Seminar, Penn State University,
  November 1989.
- 38) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
  B.H. Cooper, Bell Laboratories, General Physics Colloquium, Murray Hill, NJ,
  April 1990.
- 39) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions, B.H. Cooper, Physics Department Colloquium, University of Virginia, Charlottesville, VA, April 1990.
- 40) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions, B.H. Cooper, Charmers University of Technology, Solid State Physics Seminar, Gothenburg Sweden, June 1990.
- 41) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions,
  B.H. Cooper, Liverpool Surface Science Research Centre, Seminar, University of
  Liverpool, June 1990.
- 42) Hyperthermal Energy Ion Scattering as a Probe of Charge Transfer at Surfaces, B.H. Cooper, invited talk at the Particle-Solid Gordon Conference, Plymouth, New Hampshire, July 1990.
- 43) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions, B.H. Cooper, invited talk at the Gas-Surface Dynamics Symposium of the American Chemical Society, Washington, DC, August 1990.
- 44) Energy and Charge Transfer Mechanisms in Ion-Surface Collisions at Hyperthermal Energies,
  - B.H. Cooper, invited talk at the Workshop on Surface Reactions in the Space Environment, Evanston, Illinois, September 1990.
- 45) Ion-Surface Interactions and Scattering Dynamics,
  B.H. Cooper, General Physics Colloquium, Cornell University, December 1990.

- 46) Ion-Surface Interactions and Scattering Dynamics,
  B.H. Cooper, Colloquium, Laboratory for Research on the Structure of Matter and Department of Materials Science and Engineering, University of Pennsylvania, December 1990.
- 47) Ion-Surface Interactions and Scattering Dynamics,

  B.H. Cooper, invited talk at the Center for Chemical Physics Surface Science
  Division, National Institute of Standards and Technology, Gaithersburg, MD,
  December 1990.
- 48) Hyperthermal Na<sup>+</sup> Scattering Distributions from Cu(001): The Role of the Attractive Interaction,
  - C.A. DiRubio and B.H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 49) Cross Sections for Non-Adiabatic Resonant Charge Transfer for Li, Na, and K on Cu(001),
  - G.A. Kimmel, J.B. Marston, and B.H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 50) Non-Adiabatic Charge Transfer in O<sup>+</sup> and O<sup>+</sup><sub>2</sub> Scattering from Clean and Adsorbate-Covered Cu(001),
  - C.A. Keller and B.H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 51) A Many-Body Theory of Charge Transfer in Hyperthermal Atomic Scattering,
  J. Brad Marston, Cliff Richardson, Ernie Behringer, Greg A. Kimmel, and Barbara H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 52) Formation of Excited States in Li<sup>+</sup>-Surface Collisions Via Resonant Charge Transfer, E.R. Behringer, D. Andersson, and B.H. Cooper, contributed talk at the American Physical Society Meeting, Cincinnati, OH, March 1991.
- 53) Surface Self-Diffusion on Au(111) Observed by Scanning Tunneling Microscopy,
  D.R. Peale and B.H. Cooper, contributed talk at the American Physical Society
  Meeting, Cincinnati, OH, March 1991.
- 54) Non-Adiabatic Resonant Neutralization of Alkali Ions Scattered from Cu(100), G.A. Kimmel, J.B. Marston, and B.H. Cooper, invited talk at the European Science Foundation Workshop on Charge Transfer Phenomena at Surfaces (presented by G. Kimmel for B. Cooper), Noordwijkerhout, The Netherlands, May 1991.
- 55) Low Energy Ion-Surface Interactions,
  C.A. DiRubio, G.A. Kimmel, J.B. Marston, and B.H. Cooper, invited talk at the
  10th International Conference on Ion Beam Analysis (presented by C. DiRubio
  for B. Cooper), Eindhoven, The Netherlands, July 1991.

- 56) The Dynamics of Hyperthermal Alkali Ion-Surface Interactions,
  B.H. Cooper, D. Andersson, E.R. Behringer, C.A. DiRubio, and G.A. Kimmel, invited talk at the 12th European Conference on Surface Science (presented by E. Behringer for B. Cooper), Stockholm-Uppsala, Sweden, September 1991.
- 57) Charge Transfer and Trapping Dynamics in Hyperthermal Ion-Surface Collisions,
  B.H. Cooper, invited talk at the 6th Annual Workshop on Surface Reactions in
  the Space Environment, Evanston, Illinois, September 1991.
- 58) Multi-Channel Charge Transfer Reactions at Surfaces,
  B.H. Cooper, D. Andersson, E.R. Behringer, G.A. Kimmel, C. Keller, and J.B.
  Marston, talk at the AFOSR Molecular Dynamics Contractors Conference, Irvine,
  California, October 1991.
- 59) Dynamics of Hyperthermal Ion-Surface Collisions, March Meeting of the American Physical Society, Indianapolis, IN, March 1992, Maria-Goeppert Mayer Award Talk.
- 60) Women in Physics: The View from a Research University,

  March Meeting of the American Physical Society, Indianapolis, IN, March 1992,
  CSWP sponsored panel discussion on Women Physicists: Observations of the
  Changing Mileu Now and Then.
- 61) STM Observations of Adsorbate-Promoted Mass Flow on the Au(111) Surface, D.R. Peale, J.G. Mclean, B.H. Cooper, contributed talk at the 1992 March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 62) What Happens When Low Energy Ions Collide With Surfaces: From the Space Shuttle to Surface Processing,
  - Colgate University, Physics Department Seminar, April 1992.
- 63) What Happens When Low Energy Ions Collide with Surfaces: From the Space Shuttle to Surface Processing,
  - General Electric, Colloquium, Schenectady, NY, April 1992.
- 64) Ion-Surface Charge Transfer Dynamics,
  American Physical Society, Annual Meeting of the Division of Atomic, Molecular,
  and Optical Physics, Chicago, IL, May 1992.
- 65) Mass Flow and Stability of Nanoscale Features on Au(111): The Role of Adsorbates, DOE Sponsored Workshop on Surface Diffusion and the Growth of Materials, Santa Fe, NM, June 1992.
- 66) Charge Transfer in Ion-Surface Scattering,
  Ninth International Workshop on Inelastic Ion Surface Collisions, Aussois, France,
  September 1992.
- 67) Charge State-Resolved Scattering Measurements: Probing the Dynamics of Hyperthermal Energy Atom-Surface Interactions,

- Seventh Annual Workshop on Surface Reactions in the Space Environment, Skokie, IL, September 1992.
- 68) Positive to Negative Scattered Ion Ratios in Nonadiabatic O<sup>+</sup> Scattering from Cu(001), C.A. Keller and B.H. Cooper, March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 69) The Influence of Charge Exchange and Surface Vibrations on Hyperthermal Alkali Ion Scattering Distribution from Cu(001),
  C.A. DiRubio, G.A. Kimmel, and B.H. Cooper, March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 70) The Dynamics of Low Energy Li<sup>+</sup> Scattered from Cu(001), E.R. Behringer and B.H. Cooper, March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 71) Adsorbate Dependence of the Formation of Excited States in Alkali Ion-Surface Collision,
   D.R. Andersson, E.R. Behringer, B.H. Cooper, and J.B. Marston, March Meeting of the American Physical Society, Indianapolis, IN, March 1992.
- 72) Charge Transfer in Low Energy Collisions of Li<sup>+</sup> with Adsorbate-covered Cu(001), E.R. Behringer, D.R. Andersson, B.H. Cooper, and J.B. Marston, 52nd Physical Electronics Conference, Irvine, CA, June 1992.
- 73) Velocity Dependence of Final State Formation in Low Energy Li<sup>+</sup>-Surface Collisions, D.R. Andersson, E.R. Behringer, B.H. Cooper, and J.B. Marston, 39th National Symposium of the American Vacuum Society, November 1992, Chicago, IL.
- 74) Mass Flow and Stability of Nanoscale Features on Au(111), Fall Meeting of the Materials Research Society, Boston, MA, December 1992.
- 75) What Happens when Hyperthermal Ions Collide with Surfaces,
  Rice University, Physics Department Colloquium, Houston, TX, April 1993.
- 76) Multi-Channel Charge Transfer Dynamics in Atom-Surface Scattering, Workshop on Vibronic Processes in Gas Phase and Surface Scattering, Pousada de Palmela, Portugal, May 1993.
- 77) Energy and Charge Transfer Dynamics in Hyperthermal Energy Ion-Surface Collisions,

  Laboratoire des Collisions Atomiques et Moleculaires, Laboratory Seminar, Universite Paris-Sud, Orsay, France, May 1993.
- 78) Materials Science at a Surface,

  Cornell Materials Science Center Summer Research Experience for Undergraduate Program, Ithaca, NY, June 1993.
- 79) Ion-Surface Collisions: Probing the Dynamics of Energy and Charge Transfer, Caltech Physics Colloquium, October 1993.

- 80) Ion-Surface Interactions: Applications to Thin Film Growth,
  B.H. Cooper, talk at the AFOSR Surface Chemistry Contractor's Conference,
  Irvine, CA, October 1993.
- 81) Scanning Tunneling Microscopy for Materials Analysis,

  Cornell College of Human Ecology, Department of Textiles and Apparel Colloquium, April 1994.
- 82) Atom-Surface Interactions: Probing Dynamics with Ion Scattering,
  Brown University Physics Department Colloquium, Providence, RI, April 1994.